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Microstructure of pair centers of Cr3+-Cr2+ ions in the KZnF3 crystal

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Abstract

Studies involving the piezospectroscopy method have shown that the symmetry of the pair centers of Cr3+-Cr2+ ions in the KZnF3 crystal is tetragonal. In this paper we develop a microscopic model of a pair center. We use the temperature dependence of the integrated intensity of the absorption line to find the effective hopping integral for an eg electron, tσσ = 205 ± 10 cm-1, and the polaron reduction factor, equal to 0.11. By analyzing the selection rules for exchange-induced electric dipole transitions under double-exchange conditions we identify all the absorption lines of Cr3+-Cr2+ pairs.